

# Hadron Structure from Lattice QCD

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# Hadron Structure from Lattice QCD

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We discuss the goals and techniques of our lattice QCD calculations and explain the criteria for declaring success in this field. Based on these general considerations we have adopted a new strategy to simulate with open boundary conditions as part of the CLS collaboration. Our NIC projects form part of this large scale international effort. We illustrate our approach by showing and shortly discussing three examples, one addressing parton distribution functions (PDFs) one addressing Generalised Parton Distributions (GPDs) and one addressing Distribution Amplitudes (DAs). The upshot is that while a very detailed picture of hadron structure is emerging, reaching the required level of theoretical control will still require a long term coordinated effort.

## 1 Introduction

Particle physics is presently in a somewhat peculiar situation: On the one hand the Standard Model of the electro-weak and strong interactions is extremely successful, passing successfully one high precision test after the other, and one has all reason to be highly satisfied with its achievements. On the other hand, however, we know that there must exist Beyond the Standard Model physics (BSM). Standard quantum field theory (QFT) breaks down for energies above the Planck scale so it is clearly an incomplete theory. On the experimental side one knows from astrophysics and cosmology that dark energy and dark matter do exist, but they do not fit into the Standard Model. Seen from this perspective every successfully passed test implies that it will be still harder to learn about BSM physics. As there are limits to the energy of affordable particle accelerators (the “energy frontier”) making progress along the “precision frontier” becomes ever more important. Progress in this direction requires primarily a reduction of QCD uncertainties. In some cases this can be achieved by performing perturbative QCD calculations of ever higher order but in other cases more precise lattice simulations are needed. In fact, progress in both directions is equally important as it is always the largest individual uncertainty which determines the total. Because more and more lattice results for non-perturbative quantities cannot be tested experimentally, the complete control of the theoretical uncertainties is indispensable and actually defines success. We contribute to the continuous extension in scope and increase in precision by our lattice simulations.

Unfortunately, the level of technical sophistication in QCD has reached a point where it has become very difficult to explain to a non-expert precisely how any given example fits into the grand picture just sketched. Therefore, in this report we will focus on just three topics for which this is still relatively easy and explain these in some detail. These topics are: 1.) parton distribution functions, 2.) generalised parton distributions and 3.) distribution amplitudes.

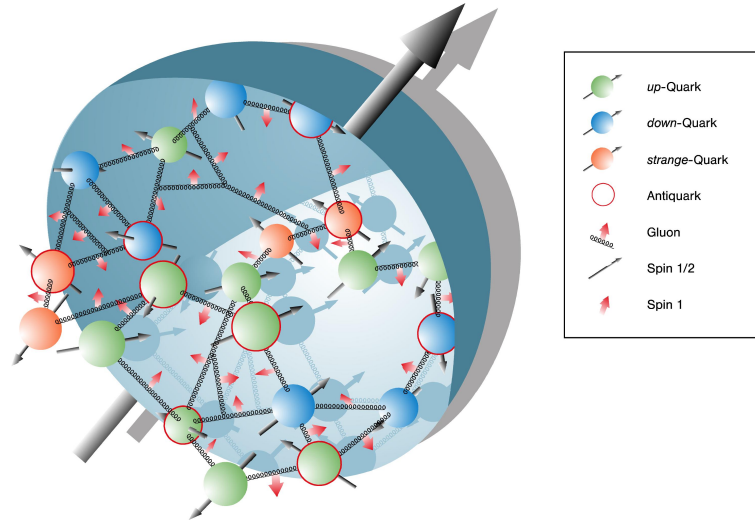


Figure 1. An illustration used by DESY to provide a feeling for the highly dynamical, fluctuating nature of the proton quantum ground state.

## 2 Fundamentals of Lattice QCD

While the hydrogen atom can be visualised quite well as being built from an electron and a proton with a mass which differs from the sum of their masses by only a fraction of  $10^{-8}$ , the sum of the valence quark masses is nearly negligible compared to the mass of, e.g. the proton, i.e. the proton mass is generated nearly exclusively by quantum mechanical interactions. Attempts to illustrate its completely quantum, highly dynamical and relativistic nature will always be a bit misleading, see Fig. 1. In reality the proton can only be described by an incredibly complicated many particle quantum wave function. Lattice QCD allows to single out and determine very specific pieces of information which are relevant for very specific experimentally observable reactions.

The first step to achieve this is to perform an analytic continuation to imaginary time. It is one of the fundamental and quite fascinating properties of QFT that this mathematically rigorously and uniquely defined operation, translates many QFT problems into purely statistical ones which can be solved numerically by Monte-Carlo techniques. Part of progress in lattice QCD is to extend the classes of objects for which this is achieved. This is highly non-trivial and requires progress in continuum QFT as well as lattice QCD and progress is, therefore, painfully slow. On the other hand any new result on fundamental interactions with a truly reliable error margin (reliable error estimates are actually the crucial distinction between theory and model building) will remain valid (within this error estimate) as long as our universe will exist. With this time perspective in mind progress in the last decades was explosive, although the impression one gets on the time scale of a PhD thesis can be somewhat different.

Fig. 2 taken from the EIC White Paper<sup>1</sup> gives a more technical illustration of what was said above. Lattice input has acquired by now a similar importance as direct experimental

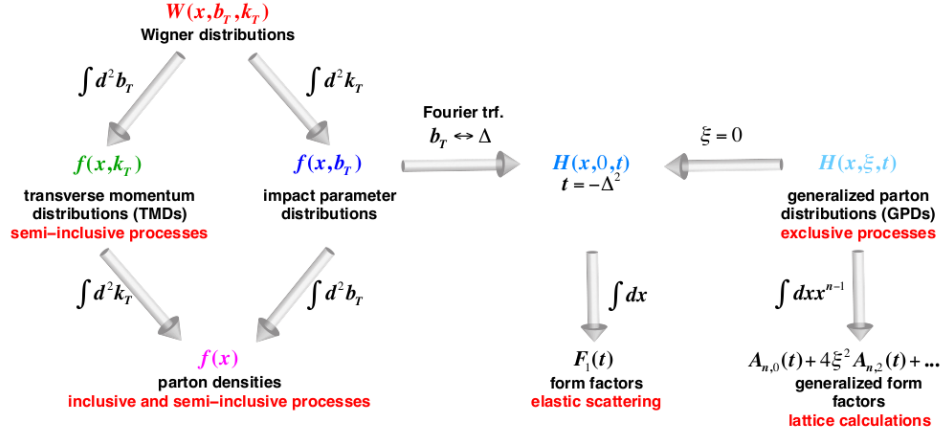


Figure 2. Part of the information characterising a hadron wave function can be expressed by Wigner distributions  $W(x, b_T, k_T)$ . Their information content can be reduced, e.g., by integrating out some variables. Experimentally, one was able to pin down several twist-2 parton densities  $f(x)$ , or rather  $f(x, Q^2)$ , and several form factors  $F(t)$ . Presently TMDs and GPDs have moved into the focus of attention. It became already clear that the purely experimental determination of all of them will hardly be possible without massive lattice QCD input to supplement experimental results. (A nucleon is, e.g., characterised by three independent types of twist-2 parton densities but eight GPDs.)

data and this might justify to invest for lattice QCD a noticeable fraction of the resources needed for such experiments.

The structure of lattice QCD calculations consists of two parts. First one generates ensembles of quark-gluon field configurations with the correct probability distributions of QCD. These ensembles can be used, in principle, to obtain all information on all hadrons. The task is then in a second step to extract very specific pieces of information, e.g., information which is related to a given experiment or a given theoretical consideration. In practice, this is limited by statistical and systematic errors. Consequently, one combines information of all ensembles at ones disposal, e.g. ensembles with various quark masses (simulations with heavier than physical masses are much cheaper) various lattice spacings and lattice volumes. Due to this constant reuse of all generated data one cannot cite all results including all future results from an individual lattice QCD project but rather one has to pick some examples as illustrations, as we do in this report. Let us add that BG computers like JUQUEEN are perfectly suited for the generation of ensembles, while, e.g., JURECA is perfectly suitable for analysis. This is why quite often we submit joint computer time proposals. It should be obvious that the needed continuous progress in hadron physics requires a continuous increase in available computer resources.

### 3 The Epic Story of $\langle x_{u-d} \rangle$

The decade long story of  $\langle x_{u-d} \rangle$  is possible best suited to illustrate the general situation described above. Twist-2 parton distributions have the great advantage to allow for a sim-

ple probabilistic interpretation while in QFT one usually has to discuss everything on the level of (interfering) probability amplitudes. For example  $u(x, Q^2)$  gives the probability that one finds an up quark with a longitudinal momentum  $xP_N^\mu$ , where  $P_N^\mu$  is the (large) 4-momentum of a nucleon, when probed, e.g., by deep-inelastic electron scattering, at a spacial resolution scale of  $1/Q$ . Such scatterings were investigated, e.g., at HERA at DESY, Hamburg. For reasons we cannot explain here the difference between the expectation value of  $x$  for up and down quarks in a proton is partially protected from higher QCD corrections and thus an especially suitable quantity for a comparison with lattice calculations. Also it is known rather precisely from experiment. Therefore, a long existing strategy is to use the uncertainties of lattice QCD calculations for  $\langle x_{u-d} \rangle$  as error estimate for all similar lattice QCD calculations. Obviously, this strategy works only, if the discrepancy between experimental and lattice QCD results is compatible with the error estimate.

As all earlier lattice calculations of  $\langle x_{u-d} \rangle$  still had substantial uncertainties, we staged a large effort to achieve unprecedented accuracy in checking this agreement. The result is shown in Fig. 3. What one can not see from this figure is that we did our very best to reduce all systematic errors and to estimate the remaining uncertainties reliably. The remaining 30% discrepancy is far too large to be ignored and in our opinion points to a fundamental problem with some present day lattice QCD calculations for hadron structure. While the cause of this discrepancy is open to debate we strongly suspect discretisation errors, i.e. artefacts due to the finite lattice spacing used. The latter is typically larger than 0.05 fm which has to be compared to a typical hadron radius of 0.7 fm. Simulations on finer lattices are not only much more expensive but also face the problem of diverging topological auto-correlation times. This problem is linked to a fundamental property of QCD. In QCD the vacuum is not an empty state, but the state of lowest energy, which has, in fact, a highly complex structure. Part of this structure is that there exist infinitely many, distinct, degenerate vacuum states differing in their topological structure. A lattice QCD calculation gives correct results if all sectors are sampled democratically. The size of artefacts if this choice is biased or if the topological sector is even fixed are unclear and heavily debated. We decided, therefore, to change our whole strategy and to switch from simulations with periodic boundary conditions to simulations with open boundary conditions, which offer the only known way to avoid the sketched topology problem. Consequently we joined the CLS collaboration which has devoted its efforts to exploring this approach. As a consequence of this decision we had to start completely from scratch generating ensembles and analysing physical observables. Meanwhile a substantial number of first preliminary results exist but they are not yet finally released. Therefore, we will rather show results obtained for the same ensembles as used for Fig. 3, which have for the stated reason not well known discretisation errors, but illustrate nicely the type of investigations we perform.

## 4 The Total Angular Momentum of Quarks in the Nucleon

The quantities displayed in Fig. 2 and others allow to answer many questions on hadron structure, although often the formal relations are rather involved and non-intuitive. (The techniques allowing to derive them are usually subsumed under the heading Operator Product Expansion (OPE).) For example a calculation which is similar to that leading to  $\langle x_{u-d} \rangle$

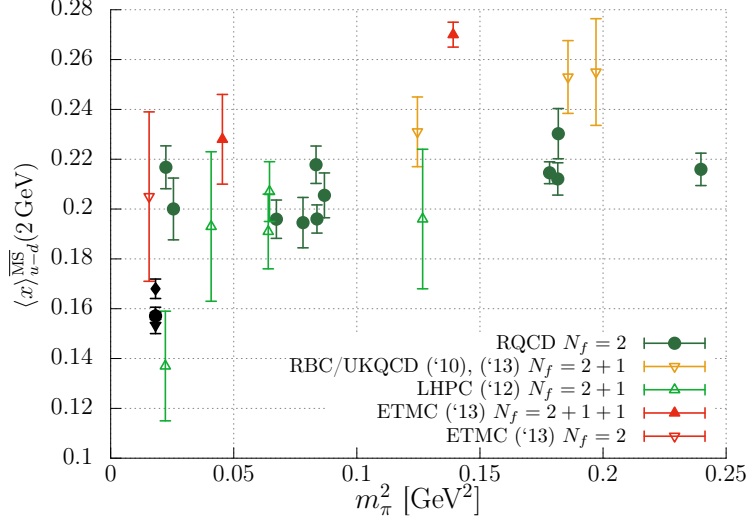


Figure 3. Results for  $\langle x_{u-d} \rangle$  from various lattice collaborations as function of the pion mass squared, which is a measure of the up and down quark mass. Physical quark masses correspond to the position of the black symbols, which show the results of phenomenological fits to experimental data. Our results are the dark green filled circles. Our lowest mass point was obtained for our largest volume.

leads to a quantity which can be identified with the total angular momentum carried by individual quark species in a proton  $J_q$ , fulfilling

$$\begin{aligned}
 J_G + \sum_q J_q &= \frac{1}{2} \\
 J^q &= \frac{1}{2} (A_{20}^q(0) + B_{20}^q(0)) \\
 &= \frac{1}{2} \int_{-1}^1 dx \, x [H(x, \xi, 0) + E(x, \xi, 0)]
 \end{aligned} \tag{1}$$

where  $H(x, \xi, 0)$  and  $E(x, \xi, 0)$  are generalised parton distributions (GPDs). Fig. 4 shows our result for the generalised form factor  $A_{20}^q(Q^2)$  for the isovector combination of valence quarks ( $B_{20}^q(Q^2)$  is not shown) and the resulting total angular momentum  $J_{u-d} = J_u - J_d$ . To obtain the error estimate, we varied every part of the analysis, fitting ranges, parametrisations as suggested by various levels of Chiral Perturbation Theory (ChPT), smearing strategies, .... This resulted in thousands of fits which we then histogrammed to read of a combined error estimate. Let us stress that moments ( $\int_0^1 dx \dots$ ) are very difficult to estimate from experimental data alone, because any experiment can only probe a limited  $x$  range.

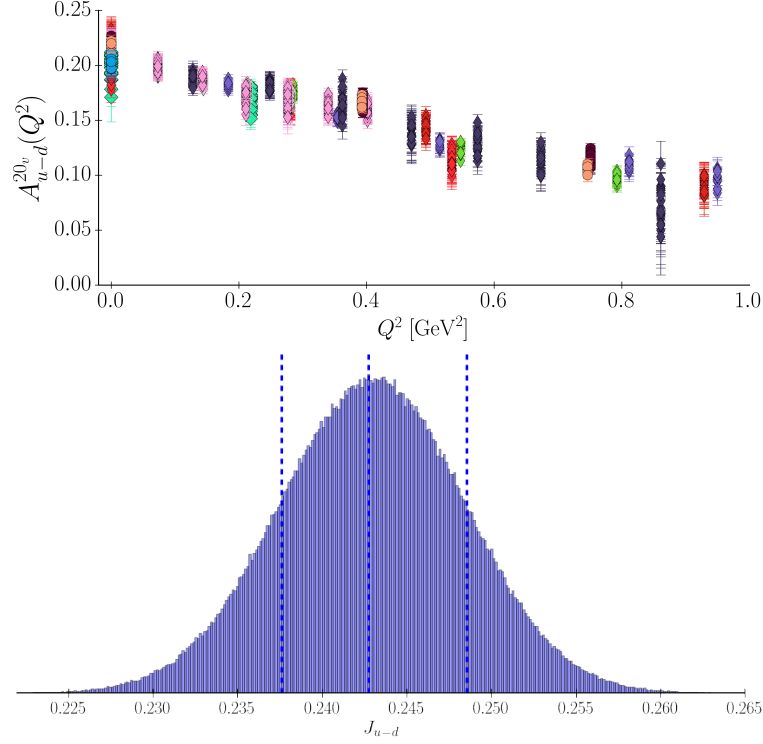


Figure 4. The generalised form factor  $A_{20}^{u-d}$  [top] and the histogram of fits for the resulting  $J_{u-d}$  [bottom]. The multiple symbols in the upper figure show the results of different fits to the primary lattice data. Very many ChPT fits to these and other similar generalised form factors resulted in the histogram in the lower figure from which we can extract a well determined fitting error.

## 5 Distribution Amplitudes

Fig. 2 comes not even close to displaying all well established elements of hadron structure. Distribution Amplitudes (DAs) contain independent information and play a pivotal role for the description of “exclusive” reactions (while distribution functions are central for “inclusive reactions”). In exclusive reactions, the 4-momenta of all participating particles are measured. In inclusive reactions this is not the case. Sufficiently hard exclusive reactions single out the properties of the leading Fock-state of a hadron multi-particle wave function. This is well known since decades, but with modern high-luminosity accelerators their precise investigation became feasible and in many respects even necessary to make full use of these machines. As the theory behind DAs is rather advanced we just show as illustration plots for the 3-quark component of the wave functions of the nucleon, the  $N^*(1535)$  and  $N^*(1650)$ . Note that the latter wave functions contain nodes. As the momentum fractions  $x_1$ ,  $x_2$  and  $x_3$  of all three quarks have to add up to 1 these wave functions can be plotted best in the manner used in that figure. We are presently preparing a paper with the DAs of the full baryon octet based on our new CLS  $N_f = 2 + 1$  ensembles for publication.

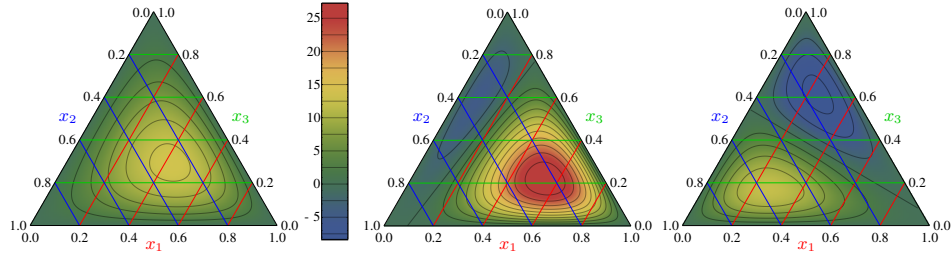


Figure 5. Barycentric plots of the nucleon [left],  $N^*(1650)$  [centre] and  $N^*(1535)$  [right] wave functions. Only the first moments of the distribution amplitude have been used to create these plots.

## 6 Algorithms

Obtaining precision results from lattice QCD poses specific challenges to software design and special algorithms are needed to achieve the needed statistical accuracy in reasonable time. The problem of topological freezing has been solved by the introduction of open boundary conditions in the time direction<sup>4</sup>. Relinquishing translational invariance in time, the method allows the topological charge to flow freely in and out of the lattice which prevents the topological charge from freezing and allows to go to finer and finer lattice spacings. The reduction in quark masses can be achieved by the use of highly efficient and parallel solvers for the inversion of the Wilson-Clover Dirac operator, employing various state-of-the-art techniques, e.g., domain decomposition and deflation. For the generation of the gauge ensembles within the CLS effort, we use a software package called “open-QCD”. It incorporates the above mentioned features like open boundary conditions and an efficient deflated solver. There are many other features that make this software very efficient, including twisted-mass Hasenbusch frequency splitting that allows for a nested hierarchical integration of the molecular dynamics at different time scales, decoupling the quickly changing but cheaper forces of the action from the more expensive low frequency part of the fermion determinant. The analysis is done with the publicly available lattice QCD software “chroma”<sup>5</sup>, steadily being extended by our group and others. E.g., recently an adaptive, aggregation based multigrid solver<sup>6</sup> has been made available, enabling us to perform inversions of the Dirac operator also at very light quark masses at low cost, see Fig. 6.

The Hierarchical Data Format (HDF5) is used to handle parallel I/O and the management of our big amounts of data. Using Data-Grid technology established by the experimental groups at the LHC we are also able to move large files in short times. By making available such technology and know-how, computer centres contribute significantly to the success of large-scale numerical efforts.

## 7 Summary

We have presented a few example for how specific information can be isolated from the complete multi-particle wave function of a hadron and related to specific experimental



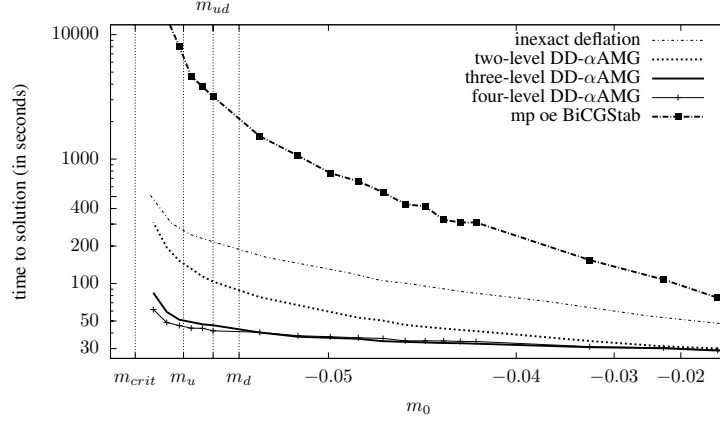


Figure 6. Time to solution for various different solvers of the Wilson-Clover Dirac operator as a function of the bare quark mass  $m_0$ . Three versions of our new algorithm resulted in the three lowest curves.

observables. We argued that to do so with really controlled errors requires a qualitative change in how lattice simulations are done, e.g., by the adaption of open boundary conditions. As part of CLS we contribute to this extensive long-term effort, using the computer time we have been granted by NIC.

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